



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1A5L / pdb_00001a5l
Title : K217C VARIANT OF KLEBSIELLA AEROGENES UREASE
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Deposited on : 1998-02-17
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

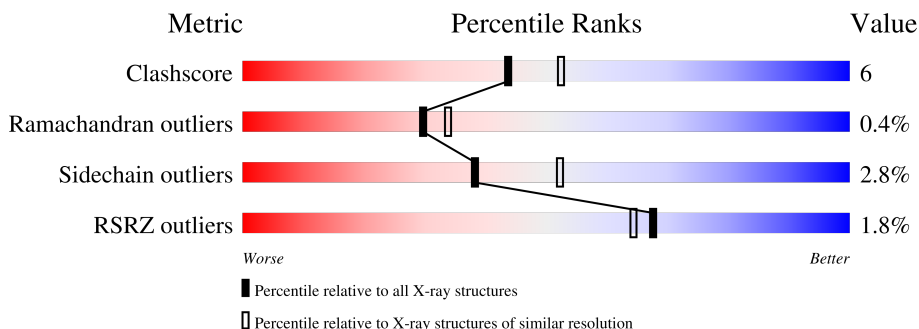
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	100	
2	B	101	
3	C	566	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5731 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UREASE (GAMMA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	0	0	0
			776	491	134	146	5			

- Molecule 2 is a protein called UREASE (BETA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			785	496	150	136	3			

- Molecule 3 is a protein called UREASE (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	536	Total	C	N	O	S	0	1	0
			3987	2502	700	764	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	217	CYS	LYS	engineered mutation	UNP P18314

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	12	Total	O	0	0
			12	12		
4	C	154	Total	O	0	0
			154	154		

- Molecule 1: UREASE (GAMMA SUBUNIT)



M1	I2	P3	G4	H7	R19	K50	E72	Q75	L81	V82	A83	R88	A89	V97	P100	L101
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S493	E345	H272	S2
L507	D346	T273	K20
R508	L348	E274	V21
R518	H349		R22
T519	S355	G277	L293
V520	L356	G278	A24
V526	S359	G279	L36
H527	D360	H280	V50
	S361	A281	C85
Y541	Q362	P282	I75
V545	A363	L284	I81
E548	G365	L285	A89
L549	V370	S296	P110
I550	L371	T298	P111
P554	L372	N299	V118
A555	R373	T301	I135
L558	V377	L302	H166
P559		P303	G173
M560	R380	T305	I177
A561	T392	L306	S178
Q562	N395	N307	R179
F567	K406	TLE	P188
	Y407	ASP	N198
	T408	GLJ	V199
	L409	HIS	S200
	N410	LEU	Q201
	P411	ASP	P202
	H419	NET	D203
		LEU	A204
		NET	L205
		VAL	V213
	N435	CYS	I218
	S436	HIS	W222
	F440	HIS	A236
	G441	LEU	V243
	V442	ASP	H246
	K443	PRD	S247
	P444	TLE	T350
	V447	ALA	
	I448	GLJ	
	K449	VAL	
	I455	ALA	
	I465	PHE	
	R474	ALA	
	P475	GLJ	
		SER	
		ARG	
		ILE	
		ARG	
		R339	

4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	170.80Å 170.80Å 170.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (10.00-2.20) 88.7 (10.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.20Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available) 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5731	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/787	0.87	0/1061
2	B	0.44	0/805	0.90	1/1087 (0.1%)
3	C	0.50	0/4071	1.02	24/5548 (0.4%)
All	All	0.49	0/5663	0.99	25/7696 (0.3%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	173	GLY	CA-C-N	9.59	129.21	119.24
3	C	173	GLY	C-N-CA	9.59	129.21	119.24
3	C	247	SER	N-CA-C	8.21	120.93	110.33
3	C	443	LYS	CA-C-N	7.83	127.76	119.85
3	C	443	LYS	C-N-CA	7.83	127.76	119.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	776	0	807	4	0
2	B	785	0	775	9	0
3	C	3987	0	3944	58	0
4	A	17	0	0	1	0
4	B	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	154	0	0	2	0
All	All	5731	0	5526	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 68 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:299:ASN:HB2	3:C:373:ARG:HD2	1.56	0.86
3:C:297:SER:HB2	3:C:349:HIS:HE1	1.44	0.82
3:C:300:PRO:HG3	3:C:364:MET:O	1.81	0.81
3:C:302:LEU:HD22	3:C:377:VAL:HG21	1.74	0.70
3:C:359:SER:O	3:C:365:GLY:HA3	1.93	0.68

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	B	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
3	C	533/566 (94%)	496 (93%)	34 (6%)	3 (1%)	21	23
All	All	730/767 (95%)	687 (94%)	40 (6%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	364	MET
3	C	481	GLY

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Mol	Chain	Res	Type
3	C	282	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/85 (100%)	84 (99%)	1 (1%)	63	78
2	B	78/78 (100%)	76 (97%)	2 (3%)	40	55
3	C	417/443 (94%)	404 (97%)	13 (3%)	35	48
All	All	580/606 (96%)	564 (97%)	16 (3%)	38	52

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	508	ARG
3	C	507	LEU
3	C	392	THR
3	C	465	ILE
3	C	372	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	486	HIS
3	C	469	GLN
3	C	349	HIS
3	C	419	HIS
3	C	201	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	100/100 (100%)	-0.74	0 100 100	3, 11, 30, 38	0
2	B	101/101 (100%)	-0.40	0 100 100	7, 18, 37, 46	0
3	C	536/566 (94%)	-0.60	13 (2%) 59 56	2, 10, 48, 85	1 (0%)
All	All	737/767 (96%)	-0.59	13 (1%) 67 64	2, 11, 41, 85	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	307	ASN	4.5
3	C	302	LEU	4.3
3	C	300	PRO	3.9
3	C	299	ASN	3.8
3	C	280	HIS	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.